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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
09/773,281	01/31/2001	Steven L. Dixon	PHARMA.002A2	1986

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EXAMINER

HIRL, JOSEPH P

ART UNIT	PAPER NUMBER
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2121

DATE MAILED: 03/17/2005

Please find below and/or attached an Office communication concerning this application or proceeding.

Office Action Summary	Application No. 09/773,281	Applicant(s) DIXON ET AL.	
	Examiner Joseph P. Hirl	Art Unit 2121	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --
Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☒ Responsive to communication(s) filed on 31 January 2001.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 1-35 is/are pending in the application.
- 4a) Of the above claim(s) _____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) _____ is/are allowed.
- 6) ☒ Claim(s) 1-35 is/are rejected.
- 7) ☐ Claim(s) _____ is/are objected to.
- 8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 29 March 2002 is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
2. ☐ Certified copies of the priority documents have been received in Application No. _____.
3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- | | |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892) | 4) <input type="checkbox"/> Interview Summary (PTO-413) |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____ |
| 3) <input checked="" type="checkbox"/> Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08) | 5) <input type="checkbox"/> Notice of Informal Patent Application (PTO-152) |
| Paper No(s)/Mail Date <u>031405</u> . | 6) <input type="checkbox"/> Other: _____ |

DETAILED ACTION

1. Claims 1-35 are pending in this application.

Double Patenting

2. A rejection based on double patenting of the "same invention" type finds its support in the language of 35 U.S.C. 101 which states that "whoever invents or discovers any new and useful process ... may obtain a patent therefor..." (Emphasis added). Thus, the term "same invention," in this context, means an invention drawn to identical subject matter. See *Miller v. Eagle Mfg. Co.*, 151 U.S. 186 (1894); *In re Ockert*, 245 F.2d 467, 114 USPQ 330 (CCPA 1957); and *In re Vogel*, 422 F.2d 438, 164 USPQ 619 (CCPA 1970).

A statutory type (35 U.S.C. 101) double patenting rejection can be overcome by canceling or amending the conflicting claims so they are no longer coextensive in scope. The filing of a terminal disclaimer cannot overcome a double patenting rejection based upon 35 U.S.C. 101.

3. Claims 1-35 provisionally rejected under 35 U.S.C. 101 as claiming the same invention as that of claims 1-35 of copending Application No. 09/770,510. This is a provisional double patenting rejection since the conflicting claims have not in fact been patented.

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Claim Rejections - 35 USC § 101

4. 35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

5. Claims 1-11 and 18-29 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter. The language of the claim raises a question as to whether the claim is directed merely to an abstract idea that is not tied to a technological art, environment or machine which would result in a practical application producing a concrete, useful, and tangible result to form the basis of statutory subject matter under 35 U.S.C. 101. Use of "computer implementation" solves this rejection.

Claim Rejections - 35 USC § 102

6. The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(e) the invention was described in (1) an application for patent, published under section 122(b), by another filed in the United States before the invention by the applicant for patent or (2) a patent granted on an application for patent by another filed in the United States before the invention by the applicant for patent, except that an international application filed under the treaty defined in section 351(a) shall have the effects for purposes of this subsection of an application filed in the United States only if the international application designated the United States and was published under Article 21(2) of such treaty in the English language.

7. Claims 1-35 are rejected under 35 U.S.C. 102(e) as being anticipated by Agrafiotis, et al (U. S. Patent 6,453,246, referred to as **Agrafiotis**).

Claims 1, 35

Agrafiotis anticipates deriving a first one-dimensional representation of a first molecule from distances between selected atoms of said first molecule (**Agrafiotis**, c 6, l 1-6; c 6, 18-20); deriving a second one-dimensional representation of a second molecule from distances between selected atoms of said second molecule (**Agrafiotis**, c 6, l 1-6; c 6, 18-20); and comparing said one dimensional representations (**Agrafiotis**, c 6, l 39-47; Examiner's Note: first molecule will have chemical properties).

Claims 2, 34

Agrafiotis anticipates said one-dimensional representations comprise linear representations (**Agrafiotis**, c 15, l 37-44).

Claim 3

Agrafiotis anticipates said deriving comprises calculating a linear position for each of a plurality of selected atoms of said first molecule (**Agrafiotis**, c 15, l 56-65).

Claim 4

Agrafiotis anticipates wherein said linear positions are selected to reduce the deviation between relative positions of said plurality of selected atoms along a line and three dimensional distances between said plurality of atoms in said first molecule(**Agrafiotis**, c 15, l 56-65).

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Claim 5

Agrafiotis anticipates calculating a linear position for each of a plurality of selected atoms of said second molecule (**Agrafiotis**, c 15, l 56-65).

Claim 6

Agrafiotis anticipates said comparing comprises aligning said one dimensional representations so as to match linear positions of at least one of said selected atoms of said first molecule with at least one of said selected atoms of said second molecule (**Agrafiotis**, c 15, l 56-65).

Claim 7

Agrafiotis anticipates said matched atoms have the same element type (**Agrafiotis**, c 12, l 58-67).

Claim 8

Agrafiotis anticipates said matched atoms have the same hybridization state (**Agrafiotis**, c 12, l 58-67).

Claim 9

Agrafiotis anticipates at least some of said distances are derived from molecular topology (**Agrafiotis**, c 14, l 1-10).

Claim 10

Agrafiotis anticipates at least some of said distances are derived from bond counts (**Agrafiotis**, c 12, l 58-67).

Claim 11

Agrafiotis anticipates at least some of said distances are derived from three dimensional atomic coordinates (**Agrafiotis**, c 15, l 37-44).

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Claim 12

Agrafiotis anticipates representing a first molecule as a first set of selected atoms, wherein each atom of said first set is associated with an atom type and a scalar value, wherein the scalar values are derived from distances between said selected atoms (**Agrafiotis**, c 6, l 1-6; c 6, 18-20); representing a second molecule as a second set of selected atoms, wherein each atom of said second set is associated with an atom type and a scalar value, wherein the scalar values are derived from distances between said selected atoms (**Agrafiotis**, c 6, l 1-6; c 6, 18-20); and comparing said atom types and scalar values (**Agrafiotis**, c 6, l 39-47).

Claims 13, 24

Agrafiotis anticipates said scalar value represents a linear position (**Agrafiotis**, c 15, l 37-44).

Claims 14, 25

Agrafiotis anticipates each atom of said set is associated with a second scalar value, said second scalar value representing a width centered about each of said linear positions (**Agrafiotis**, c 15, l 37-44; Examiner's Note (EN): seep p 11. below; width is the radius - distance to a related atom).

Claim 15

Agrafiotis anticipates wherein said comparing comprises: aligning the linear positions of an atom in the first molecule with an atom of the same type in the second molecule such that their lengths completely overlap (**Agrafiotis**, c 19, l 5-16); and evaluating the amount of overlap between atoms of the first molecule

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and atoms of the same type of the second molecule (**Agrafiotis**, c 19, l 5-16: EN: such is dissimilarity).

Claim 16

Agrafiotis anticipates repeating the aligning and evaluating steps so as to evaluate the overlap at all linearly aligned positions of atom pairs having the same type (**Agrafiotis**, c 19, l 5-16).

Claims 17, 26

Agrafiotis anticipates said second scalar value is the same for all of said selected atoms (**Agrafiotis**, c 19, l 5-16; EN: such will be the case when the atoms are the same).

Claims 18, 20

Agrafiotis anticipates representing a non-linear three dimensional configuration of a molecule made up of a plurality of bonded atoms, said method comprising assigning, to at least some of said atoms, a position along a line so as to define a set of linear distances between each of said selected atoms, wherein at least some of said linear distances are not equal to the corresponding three dimensional distances between the same atoms in said molecule (**Agrafiotis**, c 12, l 58-67; c 13, l 1-7; c 15, l 37-44; EN: topologic features are defined by three dimensions).

Claims 19, 21, 31

Agrafiotis anticipates reducing a total deviation between said set of linear distances and the corresponding three dimensional distances between the same atoms in said molecule (**Agrafiotis**, c 15, l 24-65).

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Claim 22

Agrafiotis anticipates storing linear representations of said molecular structures in a database, said linear representations being derived from three dimensional distances or topological distances between atoms of said molecular structures (**Agrafiotis**, c 15, l 56-65; Fig. 1; c 6, l 1-2); deriving a linear representation of a molecule having known biochemical activity from three dimensional distances, or topological distances between atoms of said molecule (**Agrafiotis**, c 15, l 56-65; Fig. 1; c 6, l 1-15); comparing said linear representation of said molecule having known biochemical activity with said linear representations of said molecular structures in said database (**Agrafiotis**, c 5, l 56-65; c 6, l 28-47).

Claim 23

Agrafiotis anticipates selecting a set of atoms in said molecule (**Agrafiotis**, c 6, l 1-15); deriving a set of scalar values from distances between said selected atoms (**Agrafiotis**, c 6, l 1-6; c 6, l 18-20); assigning to each of said selected atoms a parameter set including an atom type and one of said set of scalar values (**Agrafiotis**, c 15, l 56-65; EN: coordinates are parameters).

Claims 27, 28, 32, 33

Agrafiotis anticipates said distances comprise three dimensional distances (**Agrafiotis**, c 13, l 1-3; EN: topologic features are defined in three dimensions).

Claim 29

Agrafiotis anticipates comparing molecules that have been parameterized according to the method of Claim 23 (**Agrafiotis**, c 15, l 56-65).

Claim 30

Agrafiotis anticipates a computer readable storage medium having stored thereon structural representations of molecules for retrieval by a computer implemented molecular screening program, wherein at least one of said structural representations comprises a list of selected atoms in said molecule, wherein each of said selected atoms is associated with an atom type and a scalar value (**Agrafiotis**, Fig. 1 & 2; abstract; c 6, l 1-6).

Examination Considerations

8. The claims and only the claims form the metes and bounds of the invention. "Office personnel are to give the claims their broadest reasonable interpretation in light of the supporting disclosure. *In re Morris*, 127 F.3d 1048, 1054-55, 44USPQ2d 1023, 1027-28 (Fed. Cir. 1997). Limitations appearing in the specification but not recited in the claim are not read into the claim. *In re Prater*, 415 F.2d, 1393, 1404-05, 162 USPQ 541, 550-551 (CCPA 1969)" (MPEP p 2100-8, c 2, l 45-48; p 2100-9, c 1, l 1-4). The Examiner has full latitude to interpret each claim in the broadest reasonable sense. Examiner will reference prior art using terminology familiar to one of ordinary skill in the art. Such an approach is broad in concept and can be either explicit or implicit in meaning.

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9. Examiner's Notes are provided to assist the applicant to better understand the nature of the prior art, application of such prior art and, as appropriate, to further indicate other prior art that maybe applied in other office actions. Such comments are entirely consistent with the intent and spirit of compact prosecution. However, and unless otherwise stated, the Examiner's Notes are not prior art but a link to prior art that one of ordinary skill in the art would find inherently appropriate.

10. Unless otherwise annotated, Examiner's statements are to be interpreted in reference to that of one of ordinary skill in the art. Statements made in reference to the condition of the disclosure constitute, on the face of it, the basis and such would be obvious to one of ordinary skill in the art, establishing thereby an inherent prima facie statement.

11. Examiner's Opinion: p 8-10 apply. The Examiner has full latitude to interpret each claim in the broadest reasonable sense. Limitations appearing in the specification but not recited in the claim are not read into the claim. Applicant is encouraged to review all independent claims, especially those that are a distance from the enablement of the specification and incorporate appropriate limitations related to the invention.

Conclusion

12. The prior art of record and not relied upon is considered pertinent to applicant's disclosure.

- Agrafiotis et al, U.S. Patent 6,421,612
- Agrafiotis et al, U.S. Patent 6,571,227
- Agrafiotis et al, U.S. Patent 6,295,514
- Carbo et al, How Similar is one Molecule to another? An Electron Density Measure of Similarity between Two Molecular Structures

13. Claims 1-35 are rejected.

Correspondence Information

14. Any inquiry concerning this information or related to the subject disclosure should be directed to the Examiner, Joseph P. Hirl, whose telephone number is (571) 272-3685. The Examiner can be reached on Monday – Thursday from 6:00 a.m. to 4:30 p.m.

If attempts to reach the Examiner by telephone are unsuccessful, the Examiner's supervisor, Anthony Knight can be reached at (571) 272-3687.

Any response to this office action should be mailed to:

Commissioner of Patents and Trademarks,
Washington, D. C. 20231;


or faxed to:

(703) 872-9306 (for formal communications intended for entry);

or faxed to:

(571) 273-3685 (for informal or draft communications with notation of

"Proposed" or "Draft" for the desk of the Examiner).



Joseph P. Hirl

March 15, 2005